Simulating a CP-violating topological term in gauge theories

Haralambos Panagopoulos [a*] **and Ettore Vicari** [b]

[a]Department of Physics, University of Cyprus, Lefkosia, CY-1678, Cyprus
[b]Dipartimento di Fisica, Università di Pisa and INFN, I-56127 Pisa, Italy
[*]Presented the talk

E-mail: haris@ucy.ac.cy, vicari@df.unipi.it

Abstract. We present recent results on the θ-dependence of four-dimensional SU(N) gauge theories, where θ is the coefficient of the CP-violating topological term in the Lagrangian. In particular, we study the scaling behavior of these theories, by Monte Carlo simulations at imaginary θ. The numerical results provide good evidence of scaling in the continuum limit. The imaginary θ dependence of the ground-state energy turns out to be well described by the first few terms of related expansions around $\theta = 0$, providing accurate estimates of the first few coefficients, up to $O(\theta^6)$.

Four-dimensional $SU(N)$ gauge theories have a nontrivial dependence on the parameter θ which appears in the Euclidean Lagrangian as

$$\mathcal{L}_\theta = (1/4) F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) - i\,\theta\, q(x), \qquad q(x) = g^2/(64\pi^2)\,\epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x), \tag{1}$$

where $q(x)$ is the topological charge density. The ground-state energy density $F(\theta)$ behaves as

$$\mathcal{F}(\theta) \equiv F(\theta) - F(0) = (1/2)\,\chi\theta^2 s(\theta), \tag{2}$$

where χ is the topological susceptibility at $\theta = 0$,

$$\chi \equiv \textstyle\int d^4x \langle q(x) q(0)\rangle_{\theta=0} = \langle Q^2\rangle_{\theta=0}/V, \quad Q \equiv \int d^4x\, q(x), \tag{3}$$

V is the spacetime volume and $s(\theta)$ is a dimensionless even function of θ such that $s(0) = 1$. Assuming analyticity at $\theta = 0$, $s(\theta)$ can be expanded as: $s(\theta) = 1 + b_2\theta^2 + b_4\theta^4 + \cdots$, where only even powers of θ appear. Large-N scaling arguments applied to the Lagrangian (1) indicate that the relevant scaling variable in the large-N limit is $\bar{\theta} \equiv \theta/N$. This implies that in this limit $\chi = O(1)$, while the coefficients b_{2i} are suppressed by powers of N, i.e. $b_{2i} = O(N^{-2i})$.

Due to the nonperturbative nature of the θ dependence, quantitative assessments have largely focused on the lattice formulation of the theory, using Monte Carlo (MC) simulations. However, the complex nature of the θ term in the Euclidean Lagrangian prohibits a direct MC simulation at $\theta \neq 0$. Information on the θ dependence of physically relevant quantities, such as the ground state energy and the spectrum, has been obtained by computing the coefficients of the corresponding expansions around $\theta = 0$. The coefficients of $s(\theta)$ can be determined from appropriate zero-momentum correlation functions of $q(x)$ at $\theta = 0$, which are related to the moments of the $\theta = 0$ probability distribution $P(Q)$ of the topological charge Q. Indeed

$$b_2 = -\frac{1}{12\,\chi V}\left[\langle Q^4\rangle - 3\langle Q^2\rangle^2\right]_{\theta=0}, \quad b_4 = -\frac{1}{360\,\chi V}\left[\langle Q^6\rangle - 15\langle Q^2\rangle\langle Q^4\rangle + 30\langle Q^2\rangle^3\right]_{\theta=0}, \tag{4}$$

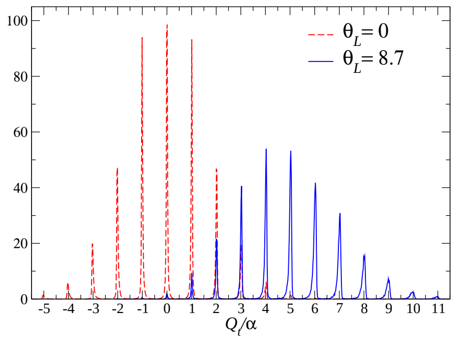

Figure 1. Distribution of the ratio Q_t/α, for $\beta = 6.2$ configurations at $\theta_L = 0$ and $\theta_L = 8.7$ ($\theta_i \approx 1.5$).

etc. They parameterize the deviations of $P(Q)$ from a simple Gaussian behavior. It has been shown that correlations involving multiple insertions of the topological charge can be defined in a nonambiguous, regularization independent way, and therefore b_{2i} are well defined renormalization group invariant quantities. The numerical evidence for a nontrivial θ-dependence, obtained through MC simulations, appears quite robust. We refer the reader to Ref. [1] for a recent review. On the other hand, MC simulations at $\theta = 0$ have only made it possible to estimate the ground-state energy up to $O(\theta^4)$. The large-N prediction $b_2 = O(N^{-2})$ has been already supported by numerical results; the calculation of the higher-order terms would provide a further check of the power-law suppression predicted by large-N arguments.

In this paper we consider imaginary values of θ, which make the Euclidean Lagrangian (1) real, thus making MC simulations possible. For further details and references, the reader may consult our Ref. [2]. Assuming analyticity at $\theta = 0$, the results provide quantitative information on the expansion around $\theta = 0$. Indeed, fits of the data to polynomials of imaginary θ may provide more accurate estimates of the coefficients, overcoming the rapid increase of statistical errors observed at $\theta = 0$. Perturbative renormalization-group (RG) arguments indicate that θ is a RG invariant parameter of the theory, thus the continuum limit should be approached while keeping θ fixed to any complex value. We find that this is indeed supported by the numerical data for the 4D SU(3) lattice gauge theory, at least for $|\theta| < \pi$, which are well described by the first few nontrivial terms of the expansion around $\theta = 0$.

Introducing the real parameter θ_i, defined by $\theta \equiv -i\theta_i$, Eq. (2) leads to:

$$\frac{\langle Q\rangle_{\theta_i}}{V} = -\frac{\partial \mathcal{F}(-i\theta_i)}{\partial \theta_i} = \chi\theta_i \left(1 - 2b_2\theta_i^2 + 3b_4\theta_i^4 + \cdots\right), \tag{5}$$

$$\frac{\langle Q^2\rangle^c_{\theta_i}}{V} \equiv \frac{\langle Q^2\rangle_{\theta_i} - \langle Q\rangle^2_{\theta_i}}{V} = -\frac{\partial^2 \mathcal{F}(-i\theta_i)}{\partial \theta_i^2} = \chi\left(1 - 6b_2\theta_i^2 + 15b_4\theta_i^4 + \cdots\right). \tag{6}$$

The nonperturbative formulation of the above theory on the lattice requires a discretization of the action, $S_L - \theta_L Q_L$; for S_L we use the plaquette gluon action, while for Q_L we employ the "twisted double plaquette" operator q_L ($Q_L = \sum_x q_L(x)$). Notice that this is not the only possible choice for q_L; the only requirement is that it have the correct continuum limit when $a \to 0$ (a: lattice spacing). In the continuum limit $q_L(x)$, being a local operator, behaves as

$$q_L(x) \longrightarrow a^4 Z_q\, q(x) + O(a^6), \tag{7}$$

where Z_q is a finite function of the bare coupling g_0, going to one in the limit $\beta \equiv 2N/g_0^2 \to \infty$. Thus, we have the correspondence: $\theta_i = Z_q\,\theta_L$, apart from $O(a^2)$ corrections. The renormalization Z_q may be evaluated by MC simulation at $\theta = 0$, computing

$$Z_q = \langle QQ_L\rangle_{\theta=0}/\langle Q^2\rangle_{\theta=0}\,, \tag{8}$$

where Q is an estimator such as those obtained by the overlap method or the cooling method, which are not affected by renormalizations, nor by nonphysical contact terms. Thus, the ratios

$$\langle Q\rangle_{\theta_i}/\langle Q^2\rangle_{\theta=0} = \theta_i - 2b_2\theta_i^3 + 3b_4\theta_i^5 + ..., \qquad \langle Q^2\rangle^c_{\theta_i}/\langle Q^2\rangle_{\theta=0} = 1 - 6b_2\theta_i^2 + 15b_4\theta_i^4 + ..., \tag{9}$$

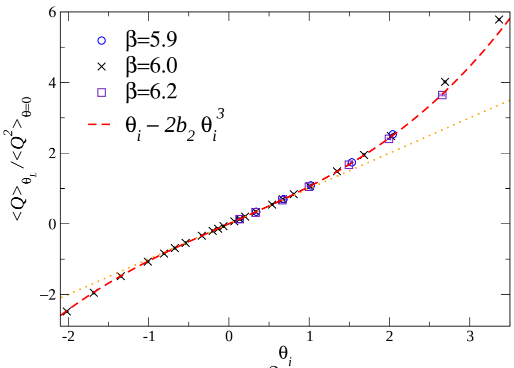

Figure 2. $\langle Q\rangle_{\theta_L}/\langle Q^2\rangle_{\theta=0}$ vs $\theta_i = Z_q\theta_L$.

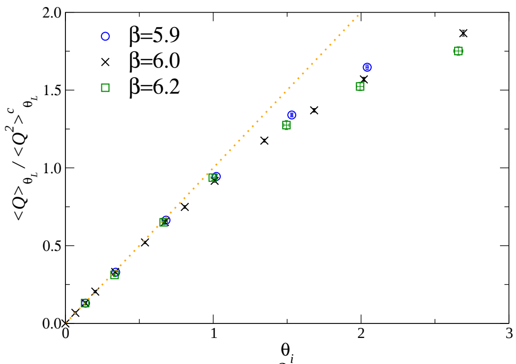

Figure 3. $\langle Q\rangle_{\theta_L}/\langle Q^2\rangle^c_{\theta_L}$ vs $\theta_i = Z_q\theta_L$.

are expected to have a well defined continuum limit as functions of θ_i .

We have carried out MC simulations of the 4D SU(3) lattice gauge theory, at $\beta = 5.9$, 6, 6.2, for lattice sizes $L = 16$, 16, 20, respectively; the simulations are carried out both at $\theta_L = 0$ and $\theta_L \neq 0$, within the region $|\theta_i| \lesssim \pi$. Since our numerical study requires high-statistics MC simulations, we choose the cooling method as estimator of the topological charge Q. The topological charge has been measured on cooled configurations (by locally minimizing the lattice action), using the twisted double plaquette operator. As is well known, this procedure leads to values $Q_t \simeq k\alpha$, where k is an integer and $\alpha \lesssim 1$. Once we determine α, we assign to Q the integer closest to Q_t/α. This cooling method for estimating Q, though less rigorous than the significantly more expensive overlap method, produces results in good agreement with it.

Fig. 1 shows the distributions of the ratio Q_t/α of $\beta = 6.2$ cooled configurations at $\theta_L = 0$ and $\theta_L = 8.7$ ($\theta_i = Z_q\theta_L \approx 1.5$). We note that these distributions cluster around integer values, also for rather large values of Q_t/α, both for $\theta_L = 0$ and $\theta_L = 8.7$.

MC simulations at $\theta = 0$ were performed at $\beta = 5.9$, 6.0, 6.2. Over 40 million sweeps per value of β were produced. The results for χ, b_2, b_4 and Z_q are reported in Ref. [2]. Providing our improved estimate of high-order coefficients, such as b_4, turned out to be very hard in $\theta = 0$ MC simulations, requiring huge statistics. The results for b_4 are consistent with zero, suggesting the bound $|b_4| \lesssim 0.005$, which is improved in $\theta \neq 0$ runs. Our estimates of Z_q (e.g. $Z_q(\beta = 6.0) = 0.135(1)$) reduce the uncertainty on Z_q as produced by other methods.

MC simulations at $\theta_L \neq 0$ are slower by approximately a factor of three, due to the complexity of the action. In $\theta_L \neq 0$ runs, ~ 3 million sweeps were produced for each value of β and θ_L. Figs. 2 and 3 show results for the ratios $\langle Q\rangle_{\theta_L}/\langle Q^2\rangle_{\theta=0}$ and $\langle Q\rangle_{\theta_L}/\langle Q^2\rangle^c_{\theta_L}$, versus $\theta_i = Z_q\theta_L$ (cf. Eq. (9)). The MC data at different β values follow the same curve, providing evidence of scaling. Scaling corrections, expected to be $O(a^2)$, are quite small, and tend to increase with increasing θ_i. This good scaling behavior corroborates the existence of a nontrivial continuum limit for any value of θ_i. Fitting our data to Eqs. (5,6,9) improves significantly the $\theta = 0$ results. In particular, a much smaller bound on b_4 is obtained: $|b_4| < 0.001$; also, we find: $b_2 = -0.026(3)$, which is clearly more precise than the estimate obtained from $\theta = 0$ runs only: $b_2 = -0.029(7)$.

Besides allowing more precise determinations of the θ expansion coefficients of the ground-state energy and other observables, using imaginary θ values might turn out useful in overcoming the dramatic critical slowing down of topological modes, by performing parallel tempering simulations with a set of θ values including θ=0; this is an *exact* MC algorithm for the model.

References

[1] E. Vicari and H. Panagopoulos, *θ dependence of SU(N) gauge theories in the presence of a topological term*, Phys. Rep. 470 (2009) 93 [`arXiv:0803.1593 hep-th`].

[2] H. Panagopoulos and E. Vicari, *The 4D SU(3) gauge theory with an imaginary θ term*, JHEP 11 (2011) 119 [`arXiv:1109.6815`].

reserved for figure